

Computational Research Division Report

OCTOBER 2007

Cosmic Alliance

A new research center focuses on computational cosmology, from supernovae to dark energy

Computational research and physics researchers gathered this month to celebrate the launch of the Computational Cosmology Center (C^3), which further cements a decade-long collaboration between two Berkeley Lab divisions for studying dark energy and other mysteries of the universe.

The two leaders of the center, Julian Borrill and Peter Nugent, jointly presented their groups' research to both the Physics and Computational Research divisions in October. Overall the Center currently comprises six researchers from the two divisions and UC Berkeley.

"Bringing a team of computational scientists from different divisions together in a single office area anticipates what we are planning to do with the new Computational Research and Theory building. The formation of the center will increase productivity and create new scientific opportunities," said Horst Simon, Associate Lab Director for Computing Sciences at Berkeley Lab. "The new center will create opportunities for scientists from both divisions to interact with each other. It will host visiting scholars who will open up new avenues for investigation in cosmology and astrophysics," said James Siegrist, Director of the Physics Division at Berkeley Lab.

The creation of C^3 comes at a time when researchers around the world are gearing up to analyze data from the European Space Agency's Planck satellite, due to launch in the summer of 2008, and begin work on the Joint Dark Energy Mission (JDEM), recently endorsed by the National Academy's Beyond Einstein Program as the top priority for the next generation space mission for NASA and DOE.

Planck, a joint ESA/NASA mission, will provide the most detailed observations to date of the Cosmic Microwave Background (CMB), the remnant radiation from the Big



Julian Borrill (left) and Peter Nugent (right) celebrated the launch of their Computational Cosmology Center with Horst Simon (middle), Associate Lab Director for Computing Sciences at Berkeley Lab.

Bang that fills the universe. Studying the tiny fluctuations in the CMB temperature and polarization will enable researchers to determine the fundamental properties of the universe with unprecedented precision.

The first detection of these fluctuations by the COBE satellite in 1992 earned Berkeley Lab's George Smoot a share of the 2006 Nobel Prize in Physics. Smoot

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Increase in Atmospheric Moisture Tied to Human Activities

Observations and climate model results confirm that human-induced warming of the planet is having a pronounced effect on the atmosphere's total moisture content, according to a study published online in the *Proceedings of the National Academy of Sciences* last month.

Using 22 different computer models of the climate system and measurements from the satellite-based Special Sensor Microwave Imager (SSM/I), atmospheric scientists, including CRD's Michael Wehner, have shown that the recent increase in moisture content over the bulk of the world's oceans is not due to solar forcing or gradual recovery from the 1991 eruption of Mount Pinatubo. The primary driver of this "atmospheric moistening" is the increase in carbon dioxide caused by the burning of fossil fuels.

"The appealing part of this study is how robust the detection of moisture changes is and that the accuracy of the satellite measurement is higher than in our previous temperature related studies," Wehner said. "This result provides a self-consistent

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STARMAN

A supernova researcher has been named a Luis Alvarez Fellow

Moving into a new dig — a larger and airy space with a window — represents a fresh start for Rollin Thomas, a new CRD researcher who will spend the next several years analyzing the physics of exploding stars.

Not that Thomas is new to Berkeley Lab. After graduating from the University of Oklahoma in 2003, Thomas joined the Nearby Supernova Factory, a collaboration among Berkeley Lab and several other institutions in the United States and France. But these days, Thomas is gear-



Rollin Thomas

ing up for a different set of challenges as a 2007 Luis W. Alvarez Fellow in Computing Sciences.

The computational science fellowship provides an opportunity for Thomas to further the work that he began at the Nearby

Supernova Factory. He has joined the

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Setting Agenda

Computing Sciences scientists to discuss research trends and findings at supercomputing conference



Researchers from Berkeley Lab's Computing Sciences will be making a significant contribution to SC07, the 20th international supercomputing conference in

Reno next month. The conference brings together scientists from national labs, universities and businesses to exchange research findings and explore trends in high performance computing.

The scientists, from CRD, NERSC and ESnet, will hold workshops and discussions, as well as presenting their research. Some will carry out technical demonstrations. Many of their works will be published in the conference journal, the *Proceedings of Supercomputing (SC07)*.

"The conference is a great venue to highlight the expertise of our researchers, who are contributing to nearly 10 percent of all the papers accepted for the journal," said Horst Simon, Associate Lab Director for Computing Sciences. "They also influence dialogues and research trends in computing sciences through hosting workshops and other discussions."

Here is a list of researchers who are holding workshops:

- Andrew Canning will co-host the "Third International Workshop on High Performance Computing for Nanoscience and Nanotechnology (HPCNano07)." Lin-Wang Wang and Osni Marques also will speak at the workshop.
- Erich Strohmaier will present an analysis of this year's TOP500 list and discuss trends in the high performance computing marketplace during a Birds of a Feather (BOF) session.
- John Shalf and Erich Strohmaier will host a BOF session on "Power, Cooling and Energy Consumption for Petascale and Beyond."
- Bill Kramer is one of the organizers for the "Petascale Data Storage Workshop."
- Phil Colella will co-host a BOF discussion on "Federal Activities Impacting Long Term HEC Strategies."

Scientists to present papers are:

- Julian Borrill, Lenny Oliker, John Shalf and Hongzhang Shan will discuss their work on the "Investigation of Leading HPC I/O Performance Using a Scientific Application-Derived Benchmark."
- Parry Husbands and Kathy Yelick will present "Multithreading and One-Sided Communication in Parallel LU Factorization."
- Sam Williams, Lenny Oliker, Kathy Yelick, Rich Vuduc, Jim Demmel and John Shalf will talk about their paper, "Optimization of Sparse Matrix Vector Multiplication on Emerging Multicore Architectures."
- Phil Colella, Kathy Yelick and Noel Keen, along with Tong Wen from IBM Research and Jimmy Su from UC Berkeley, will present "An Adaptive Mesh Refinement Benchmark for Modern Parallel Programming Languages."
- Erich Strohmaier co-authored a paper titled, "A Genetic Algorithms Approach to Modeling the Performance of Memory-Bound Computations."

Zhengji Zhao, Juan Meza, and Lin-Wang Wang will present a poster, "A New O(N) Method for Petascale Nanoscience Simulations."

Kathy Yelick, head of CRD's Future Technologies Group, Paul Hargrove and two graduate students, Dan Bonachea and Rajesh Nishtala, all from the same group, will be manning a booth called "PGAS: Partitioned Global Address Space Programming Paradigms."

ESnet staff will carry out networking demonstrations that showcase its on-going effort to significantly boost the science network's bandwidth and services for DOE researchers and their collaborators. Chin Guok and Eli Dart will lead the demonstrations.

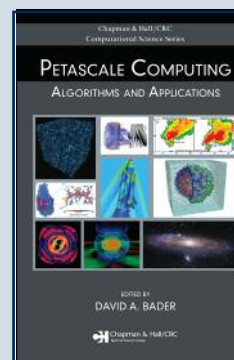
Computing Sciences staff also worked on committees to organize various components of the conference. Participants who are coming from NERSC are Bill Kramer, NERSC's General Manager, who serves on the Steering Committee for the conference; Harvey Wasserman, who chairs the Technical Program Committee;

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Hall of Fame

Read This Book

Researchers at Berkeley Lab's Computing Sciences co-wrote several chapters of an upcoming book



on petascale computing. The book launch will take place at SC07 in Reno next month.

The book, "Petascale Computing: Algorithms

and Applications," is the first in the Chapman & Hall/CRC Computational Science Series. Horst Simon, Associate Lab Director of Computing Sciences, which includes CRD and NERSC, serves as the series editor. David Bader of Georgia Institute of Technology edited the first book.

Content for the book came from a 2006 workshop at Schloss Dagstuhl.

In the book's introduction, Simon notes that book summarizes "the state of knowledge in algorithms and applications in 2007, just before the first petascale systems will become available. Just like petascale computing will open up new and unprecedented opportunities for research in computational science, I expect this current book to lead the new series to a deeper understanding and appreciation of research in computational science and engineering."

The Computing Sciences researchers who have contributed to the book include John Shalf, Lenny Oliker, Michael Lijewski, Shoaib Kamil, Jonathan Carter, and Andrew Canning, all of whom co-wrote the first chapter, called "Performance Characteristics of Potential Petascale Scientific Applications."

Erich Strohmaier wrote Chapter
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Computational Cosmology *continued from page 1*

was also the principal investigator of the Laboratory Directed Research and Development (LDRD) project that brought Borrill to NERSC in 1997 specifically to develop the high performance computing tools needed to analyze CMB data sets like Planck's.

The study of Type Ia supernovae marks the other key area of research by the C³ group. Researchers' ability to calibrate their brightness to just a few percent provides an excellent yardstick for measuring distances across the universe. These supernovae are fundamental in measuring the expansion history of the universe and are utilized in all the proposed JDEM missions to date. Researchers first found proof that the expansion of the universe is accelerating — not slowing down as many experts had believed — by poring over data of far-away Type Ia supernovae.

Nugent was on one of the two international teams, led by Saul Perlmutter of Berkeley Lab, that announced the discovery independently in 1998. Nugent also is a member of the SciDAC Computational Astrophysics Consortium, which is funded by the DOE Office of Science to develop scientific computing software for carrying out large-scale research of supernovae, gamma ray bursts and nucleosynthesis.

"High performance computing will be critical for the simulations and data analysis that will be needed to understand dark energy," said Borrill. Using the new capabilities afforded by NERSC's recently acquired Franklin supercomputer, Borrill and colleagues have recently performed



Leaders within Computing Sciences gathered for the toast. From left, Bill Johnston, head of ESnet; Kathy Yelick, Director of NERSC; Horst Simon, Associate Lab Director for Computing Sciences; Francesca Verdier, an Associate General Manager of NERSC.

the first simulation and analysis of a year of data from all of Planck's detectors in an effort to test different codes and ready them for analyzing the real data later.

Nugent has been working on the Nearby Supernova Factory data analysis as part of his SciDAC collaboration. As a byproduct of this work, he has assembled all the historical imaging taken at the Palomar Oschin Schmidt telescope over the past seven years that has been used for hunting for supernovae. The entire 60-terabyte dataset creates both a temporal and static catalog of astrophysical objects.

"I was in the unique position of utilizing my expertise in astrophysics imaging and linear algebra coupled with my parallel processing knowledge to work this through on the NERSC machines," Nugent said.

Nugent's work has attracted the attention of many groups and will form a very useful dataset for the entire astrophysical community.

Aside from Nugent and Borrill, other C³ members are Chris Cantalupo, Ted Kisner, Rollin Thomas and Sebastien Bongard. Thomas was recently named a Luis Alvarez Computational Science Fellow.

Hall of Fame *continued from page 2*

16, titled "Performance and Its Complexity on Petascale Systems."

Shalf also is a co-author of Chapter 24, "Cactus Framework: Black Holes to Gamma Ray Bursts."

A book launch party is scheduled to take place at Georgia Tech's SC07 booth from 10:30 a.m. to 11 a.m. on November 13.

The booth, 3221, can be found on the [SC07 map](#). You can find the book at the [CRC Press](#).



Horst Simon

UC Appointment

Horst Simon, Associate Lab Director for Computing Sciences, has been named as an adjunct professor in the Department of Electrical Engineering and Computer Science (EECS) at UC Berkeley.

"I'm very pleased by this appointment and see it as another link in

bringing LBNL Computing Sciences and the computer science program on campus even closer together," Simon said.

He added that he is working with EECS professor Jim Demmel and Dean Mark Richards of Cal's Division of Physical Sciences to develop a "designated graduate emphasis in computational science and engineering." Demmel also is a CRD researcher.

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Atmospheric Moisture *continued from page 1*

picture of a planet both warmed and moistened by human activities. Hence, our confidence in predictions of future man-made global warming is increased."

More water vapor — which is itself a greenhouse gas — amplifies the warming effect of increased atmospheric levels of carbon dioxide. This is what scientists call a "positive feedback."

"When you heat the planet, you increase the ability of the atmosphere to hold moisture," said Benjamin Santer, lead author from Lawrence Livermore National Laboratory's Program for Climate Modeling and Intercomparison. "The atmosphere's water vapor content has increased by about 0.41 kilograms per square meter (kg/m^2) per decade since 1988, and natural variability in climate just can't explain this moisture change. The most plausible explanation is that it's due to the human-caused increase in greenhouse gases."

The study is the first "fingerprint" study on the amount of water vapor in the atmosphere.

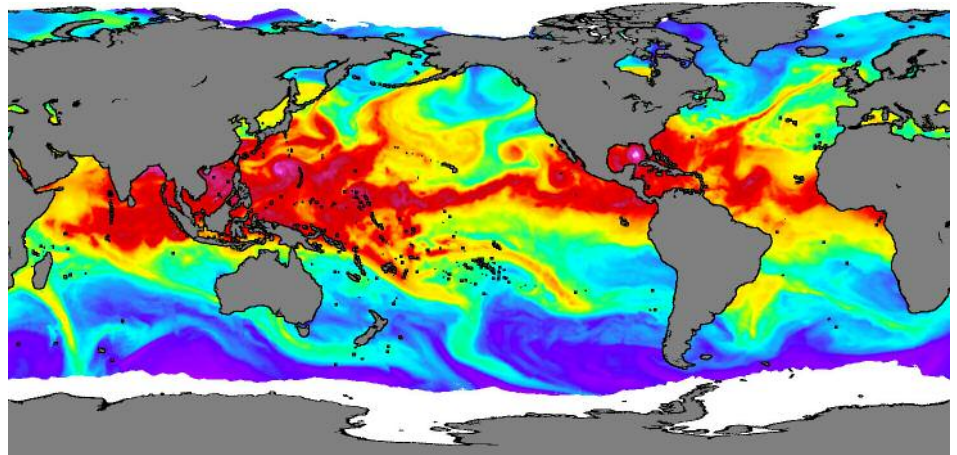
"Fingerprint" studies seek to identify the causes of recent climate change and involve rigorous comparisons of modeled and observed climate change patterns. To date, most fingerprint studies have focused on temperature changes at the Earth's surface, in the free atmosphere or in the oceans. Or they have considered variables whose behavior is directly related to changes in atmospheric temperature.

The water vapor feedback mechanism works in the following way: as the atmosphere warms due to human-caused increases in carbon dioxide, methane, nitrous oxide, and chlorofluorocarbons, water vapor increases, trapping more heat in the atmosphere, which in turn causes a further increase in water vapor.

Basic theory, observations and climate model results all show that the increase in water vapor is roughly 6 percent to 7.5 percent per degree Celsius warming of the lower atmosphere.

The authors note that their findings, when taken together with similar studies of continental-scale river runoff, zonal-mean rainfall, and surface specific humidity, point toward an emerging human-caused signal in the cycling of moisture between the atmosphere, land and ocean.

"This new work shows that the climate



Estimates of the amount of atmospheric water vapor over oceans from the satellite-based Special Sensor Microwave Imager. Results are from August 28, 2005. Locations with high atmospheric moisture content are denoted by red and white colors. The highest water vapor values are associated with typhoons Talim and Nabi in the Pacific and with Hurricane Katrina in the Gulf of Mexico. Image credit: Carl Mears and Frank Wentz/Remote Sensing Systems

system is telling us a consistent story," Santer said. "The observed changes in temperature, moisture, and atmospheric circulation fit together in an internally and physically consistent way."

Other scientists contributing to this research were Karl Taylor, Peter Gleckler, Jim Boyle and Stephen Klein from Livermore Lab; Carl Mears and Frank Wentz at Remote Sensing Systems in Santa Rosa, Calif.; Tom Wigley, Jerry Meehl, and Warren Washington at the National Center for Atmospheric Research

in Boulder; Tim Barnett and Dave Pierce at Scripps Institution of Oceanography in La Jolla; Wolfgang Brüggemann at the University of Hamburg in Germany; Nathan Gillett at the University of East Anglia and Peter Stott at the Hadley Centre for Climate Prediction and Research (both in the U.K.); Toru Nozawa at the National Institute for Environmental Studies in Japan.

You can read the full research paper at <http://www.pnas.org/cgi/content/full/104/39/15248>.

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Scott Campbell and Jason Lee, who serve on SCinet's Network Monitoring Committee. Cary Whitney is on SCinet's Open Fabrics Committee. Zaida McCunney and Lynn Rippe serve on the committee for the Learning & Physical Challenges Education Program.

CRD staff who serve on committees are Esmond Ng, head of CRD's Scientific Computing Group, who is on the technical program's Applications Program Committee. He also sits on the Sidney Fernbach Memorial Award Committee. Craig Leres serves on SCinet's Fiber Committee. Keith Jackson is on the Grid Program Committee. Lenny Olikar is on the Performance Committee. George "Chip" Smith is part of the Cluster Challenge Committee. Erich

Strohmaier is a Doctoral Research Showcase PC member. Jon Bashor serves as the liaison to the Communications Committee at the conference. Eli Dart from ESnet is on SCinet's Routing Committee.

David Bailey, CRD's chief technologist, chairs both the Gordon Bell Prize Committee and the Seymour Cray Award Committee.

George Smoot, winner of the 2006 Nobel Prize in Physics and a Berkeley Lab researcher, will be a keynote speaker. William Tschudi, a researcher from the Environmental Energy Technologies Division at Berkeley Lab, will be on a panel called "Is There an HEC Energy Crisis?"

Check out SC07's technical program at <http://sc07.supercomputing.org/?pg=tech-program.html>.

Rollin Thomas *continued from page 1*

newly formed Computational Cosmology Center, which brings together scientists in the Computational Research Division and Physics Division.

"He received his Ph. D. at the University of Oklahoma in physics with a concentration in astronomy and has extensive computational expertise in massively parallel supernova simulations," said Peter Nugent, who is co-leading the center with Julian Borrill.

Thomas will work closely with Nugent, who also received his Ph.D. in physics, with a concentration on astronomy, from the University of Oklahoma, as well as Dan Kasen, a Hubble Fellow at UC Santa Cruz.

The center bridges theory and experiment in supernova research. The theorists develop computational tools and use supercomputers to model supernovae, while scientists on the other side look for empirical relations among observational data.

"Somewhere in between, there are people who have to reconcile the models with the observations — that's where I live," said Thomas, who will use supercomputing resources at NERSC to develop techniques for analyzing the large amount of data collected by the Nearby Supernova Factory.

His attraction to objects in the sky started when he was a boy. Thomas got his first telescope for Christmas in 1981, when he was in the first grade. The refractor telescope brought him a close-up look of the moon and Venus and a life-long love for learning about the universe.

Watching the night sky wasn't the only hobby for the young Thomas. He also spent a lot of time in front of a computer. The two interests would pave the way for him to pursue the field of computational astrophysics later on.

Thomas attended Purdue University, where he graduated with a bachelor's degree in physics in 1997. While studying physics, he also studied Russian. He enjoyed learning foreign languages and took German and Spanish in high school. "They were fun — I had a knack for it," Thomas said.

In fact, he flirted with the idea of becoming a linguist. But a linguist doesn't earn much money, and being an astrophysicist still held a strong appeal. Then in 1996,

he met David Branch, a professor at the University of Oklahoma who would become his dissertation advisor.

Well loved by students partly for his willingness to let them be lead authors of scientific papers, Branch introduced Thomas to the world of supernovae.

"I really liked going to talk to him," Thomas recalled. "He didn't have to try very hard to convince me to go to graduate school at Oklahoma."

It was an exciting time to jump into the supernova research. Scientists around the world were racing to answer a big question: Is the universe expanding at a slower pace than before? Many researchers thought

At the end of the day, we want to find the correlations between certain spectroscopic features and shapes and how they correlate with the brightness of a supernova.

— Rollin Thomas, Luis Alvarez Fellow

so. It wasn't until 1998 that two international teams of scientists independently demonstrated that the expansion was in fact accelerating. Nugent was on one of the teams, led by Berkeley Lab's Saul Perlmutter.

The breakthroughs wouldn't have been possible without using data about a class of exploding white dwarf stars called Type Ia. The Type Ia supernovae are good tools for measuring cosmological distance because they have a known luminosity, the amount of energy radiated over time. As the universe expands, the brightness begins to dim to observers on Earth, and the light's wavelength starts to shift toward the red end of the spectrum.

But more work needs to be done to better understand the brightness and other features of the supernovae, research that would make Type Ia an even more precise measurement for determining the rate of the universe's expansion. That's the mission of the Nearby Supernova Factory, which had just gotten started when Thomas joined in 2003.

Thomas worked on amassing those observational data from the 1.2-meter tel-

escope at the Palomar Observatory in Southern California. He also helped to collect the follow-up spectroscopic data from the 2.2-meter telescope at Mauna Kea in Hawaii. Because such stellar explosions only take place a few times per millennium in each galaxy, scientists are keen on capturing those rare occurrences.

These days, the Nearby Supernova Factory, led by Greg Aldering, is a rich depository of the Type Ia supernova data.

"Scientists for the most part have concentrated on studying the individual supernovae they were fortunate to observe in detail," Thomas said. "That is still important, but we can apply more powerful tools to a much larger, more homogenous data set like the few thousand observations obtained by the Nearby Supernova Factory." With an interest in spectroscopy, Thomas will focus on developing computer models of radiation and its interaction with matter as the Alvarez Fellow.

"At the end of the day, we want to find the correlations between certain spectroscopic features and shapes and how they correlate with the brightness of a supernova," Thomas said. "Then you can have an independent means of measuring how bright it is and use it as a cosmic distance indicator."

When Thomas isn't working on unraveling the mystery of the universe, he can be found hanging out at museums with his wife, Dianna LaFerry, who graduated with an art degree from the University of Oklahoma and owns a business designing sewing patterns and digital illustrations.

About CRD Report

CRD Report, which publishes every other month, highlights the cutting-edge research conducted by staff scientists in areas including turbulent combustion, nano materials, climate change, distributed computing, high-speed networks, astrophysics, biological data management and visualization. CRD Report Editor Uclia Wang can be reached at 510 495-2402 or Uwang@lbl.gov. Find previous CRD Report articles at <http://crd.lbl.gov/html/news/CRDreport.html>.

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Julian Borrill

Astrophysicist Joins NASA Team

Julian Borrill, an astrophysicist in the Scientific Computing Group, has been invited to join NASA's Primordial

Polarization Program Definition Team (PPPDT), charged with planning the cosmic microwave background radiation (CMB) polarization mission after the upcoming Planck satellite mission.

The team includes 13 experimentalists (including the PIs of two other major CMB missions, WMAP and US Planck), one theorist and one data analyst.

"The presence of even one data analyst is an enormous step forward, and reflects the growing recognition of the need to include data analysis in CMB mission planning and the critical role that NERSC and LBNL play in the field," Borrill said.

Borrill, along with Chris Cantalupo and Ted Kisner, has been doing extensive simulations based on the amount of data expected to be gathered over the course of a year by the 74 detectors on Planck satellite.

Members of the PPPDT will work in collaboration with NASA headquarters, the National Science Foundation (NSF), DOE, NASA field center scientists and engineers and the astronomical community to provide input during conceptual development of a CMB polarization mission. The PPPDT will help provide the astronomy community input on questions relating to the science capabilities of a potential mission and will help disseminate information about the mission concept to the community. See <http://groups.physics.umn.edu/cosmology/PPPDT> for more details.



Daniela Ushizima

New Staff

Daniela Ushizima has joined Computing Sciences at Berkeley Lab after spending two years as an assistant professor at the Catholic University of Santos in

Brazil.

Ushizima will split her time between the Mathematics and Visualization groups in the Computational Research Division. The Visualization group also serves as the Analytics Team at NERSC.

She earned a Ph.D. in Applied Physics on Computing Vision from the University of Sao Paulo's Physics Institute of Sao Carlos in 2004, after she obtained a master's degree at the same institute. Ushizima graduated from the Federal University of Sao Carlos in Brazil with a bachelor's degree in Computer Science in 1997. She was also a visiting researcher in the Electrical and Computer Engineering Department at UC Santa Barbara in 2004.

While at the Catholic University of Santos, Ushizima taught in the Master's Degree Program as a member of the Intelligent Systems Group in the Department of Informatics. She led several government projects funded by the Fundação de Amparo à Pesquisa do Estado de São Paulo (Foundation for Research Support of the State of São Paulo, or FAPESP). From 2005 to 2007, she led the work on Computer Vision in leukemia diagnosis.

Ushizima also served as an industry consultant for several companies in Brazil, including Natcomps, Fleury Institute of Clinic Analysis and Ablevision.

Sefa Dag has joined CRD's Scientific Computing Group as a post-



Sefa Dag

doctoral fellow. He will be working with Lin-Wang Wang in organic/inorganic interfaces and electronic structure of organic systems. In particular, Dag will study how the charge

patching method can be applied to inorganic molecules, what the atomic structures of organic/inorganic interfaces are, and what the electron conductivity in an organic polymer is.

Sefa received his Ph.D. from Bilkent University in Ankara, Turkey. Prior to coming to LBNL, Sefa was a postdoctoral fellow in the Computer Science and Mathematics Division and the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory. He has extensive experience in large-scale electronic structure calculations and material simulations, e.g., for carbon nanotubes and metal oxide surfaces.



Anurag Chaudhry

Anurag Chaudhry, a Ph.D. student at UC Davis, has joined CRD's Scientific Computing Group. Andrew Canning and Niels Jensen serve as his thesis advisors.

Anurag is currently involved in a life sciences project at Berkeley Lab called "High-Throughput Discovery of Improved Scintillation Materials," for which Steve Derenzo from the Lab's Life Sciences Division is the lead principal investigator and Canning is the principal investigator for theory.

Anurag is a guest in SCG working with Andrew Canning. He will be performing first principles simulations of cerium-doped materials to determine their brightness for gamma ray detection. Anurag received his Master's degree from the Indian Institute of Technology in Delhi, India.

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